Butanamide, 4-hydroxy-

927-60-6 | DTXSID5061297

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 8.36e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.35e-01

Confidence level: 8.17e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl lactate
Measured: 3.90e-12
Predicted: 4.80e-12

Image not found
2-Ethoxyethyl acetate
Measured: 1.30e-11
Predicted: 1.03e-11

Image not found
Ethyl 3-ethoxypropionate
Measured: 2.29e-11
Predicted: 1.63e-11

Image not found
Methyl 2-hydroxypropanoate
Measured: 2.80e-12
Predicted: 3.16e-12

Image not found
2-Ethoxyethyl isobutyrate
Measured: 1.35e-11
Predicted: 1.28e-11